Special Topics on Basic EECS I
VLSI Devices
Lecture 2

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1D space with a flat potential (Free electron)

- Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

  - Periodic boundary condition, $\psi(0) = \psi(Na)$.
  - Its solution

$$\psi(x) \propto \exp\left(i\frac{2\pi}{Na}nx\right) = \exp ikx$$

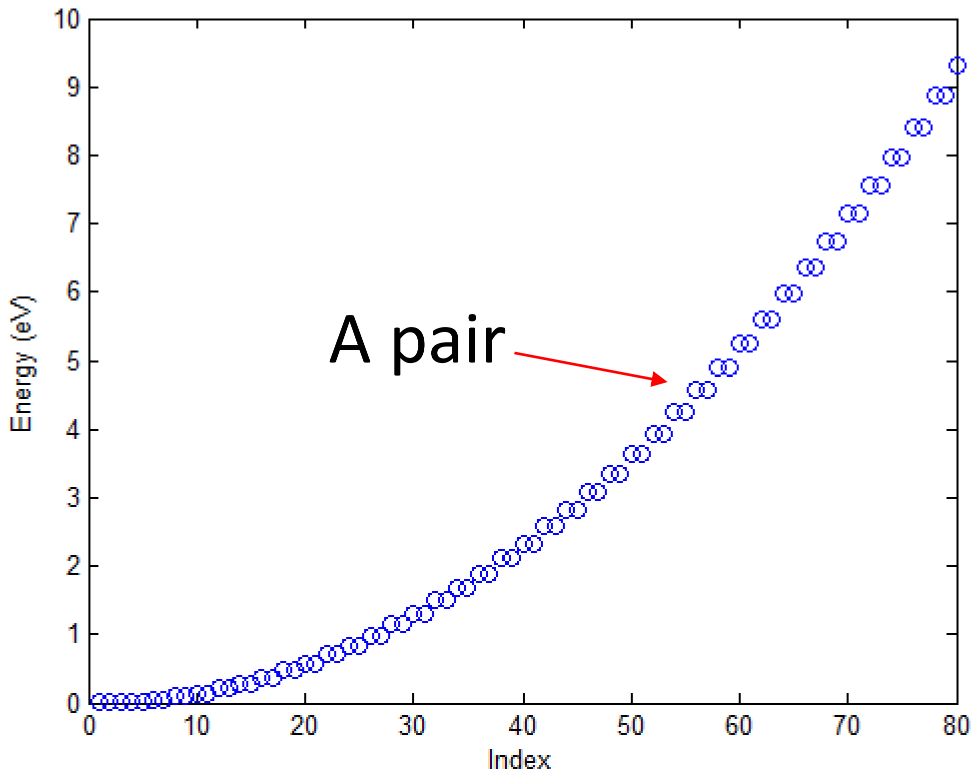
Plane wave

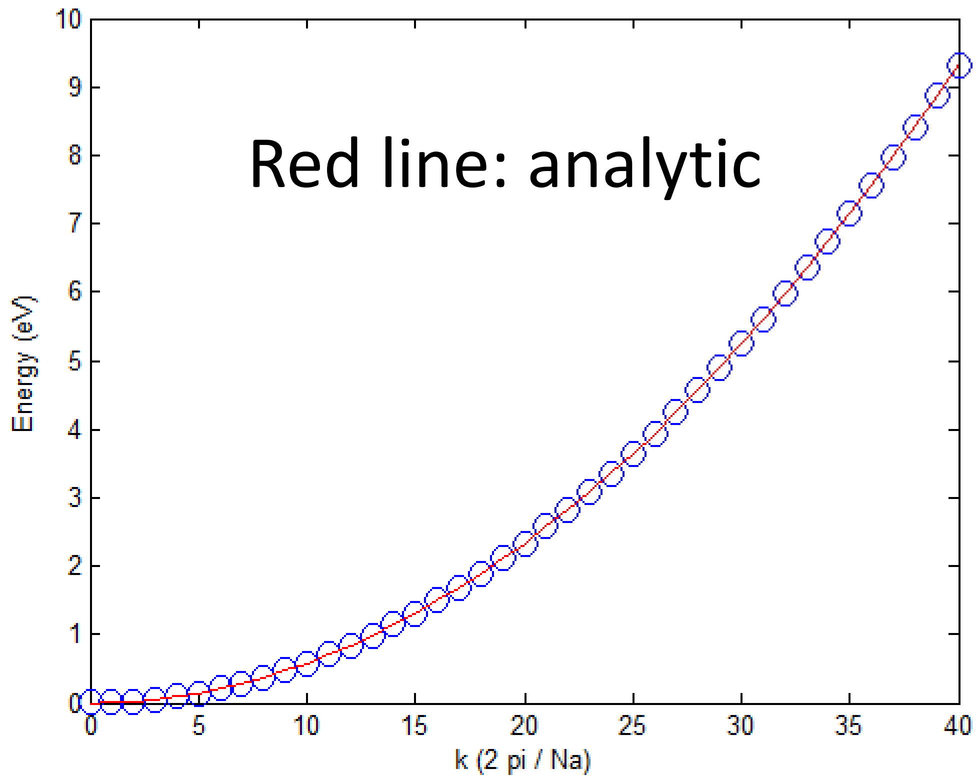
$$E = \frac{\hbar^2}{2m}k^2$$

  - k can be used to identify a state.

Numerical example (Free electron)

- When a is 0.4 nm and N is 40,
  - 80 states with lowest energies

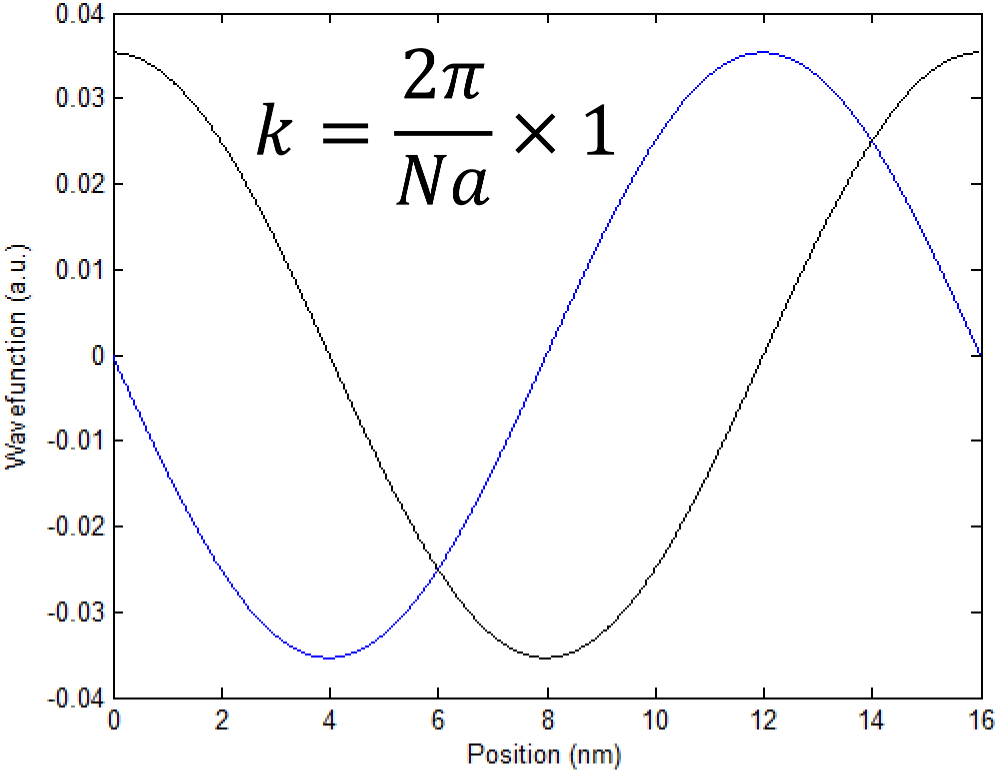


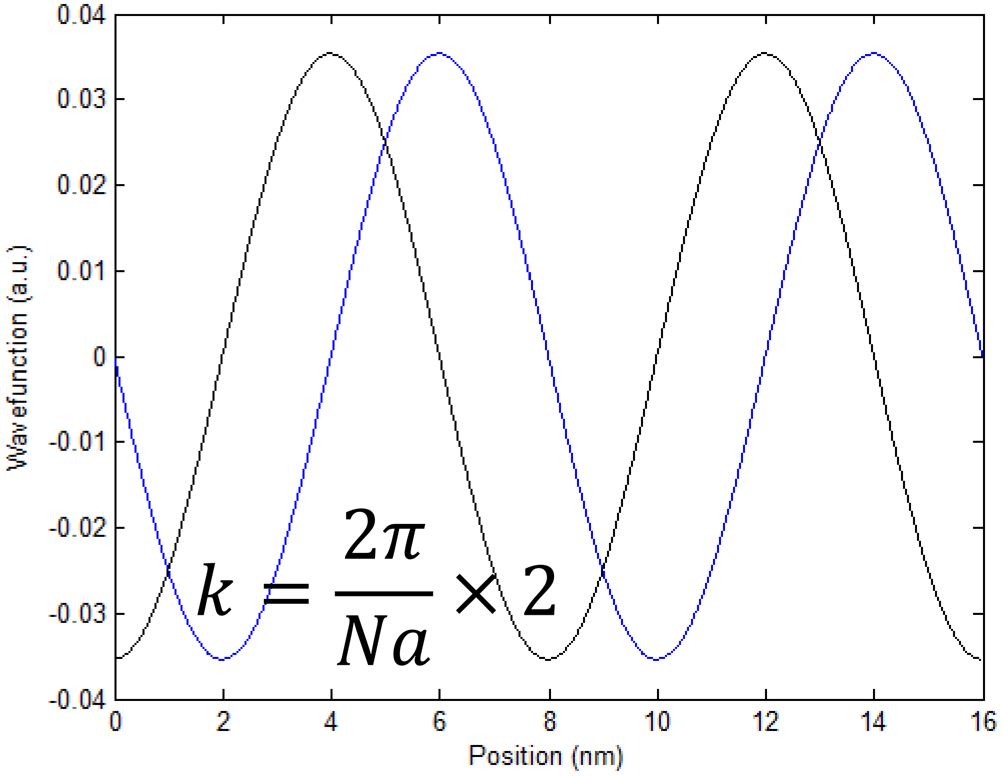


Pair?

- Two sinusoidal wavefunctions with the same period

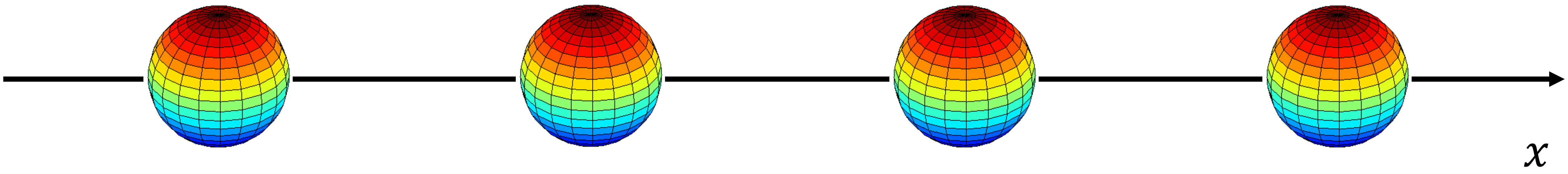
$$\exp ikx = \cos kx + i \sin kx, \exp(-ikx) = \cos kx - i \sin kx$$





Periodicity

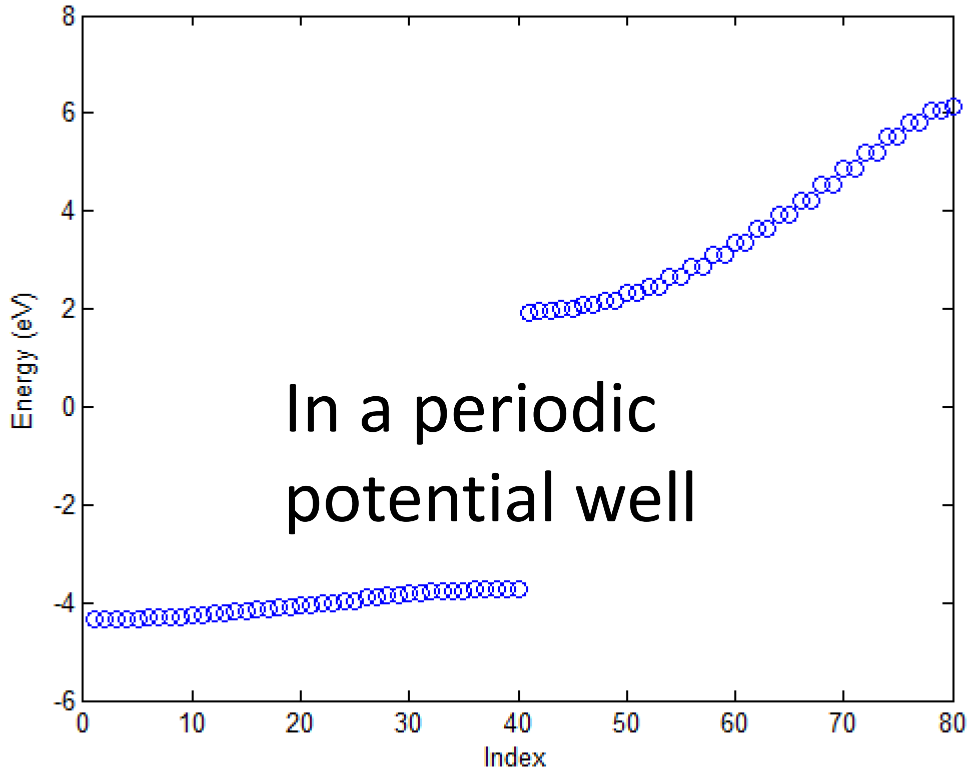
- Atoms are placed in a periodic manner.
  - They are attracting electrons. (Negative potential)

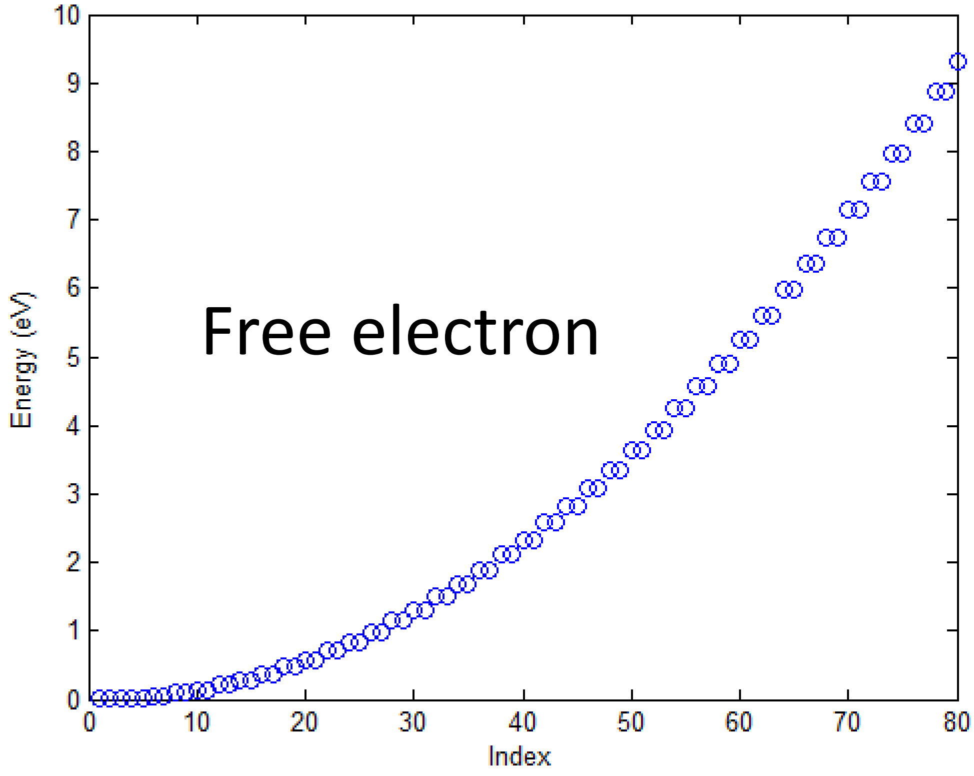


  - Let us consider a periodic potential well.

Numerical example (Periodic potential well)

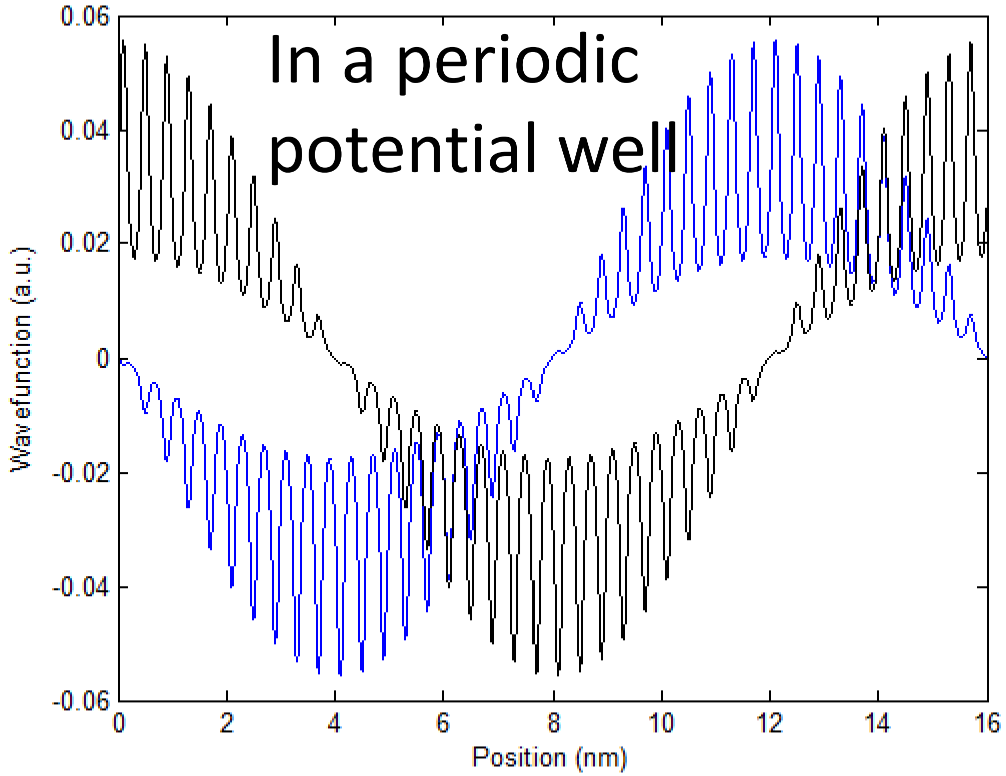
- When a is 0.4 nm, N is 40, the well width is 10 nm, and the well depth is 10.0 eV,

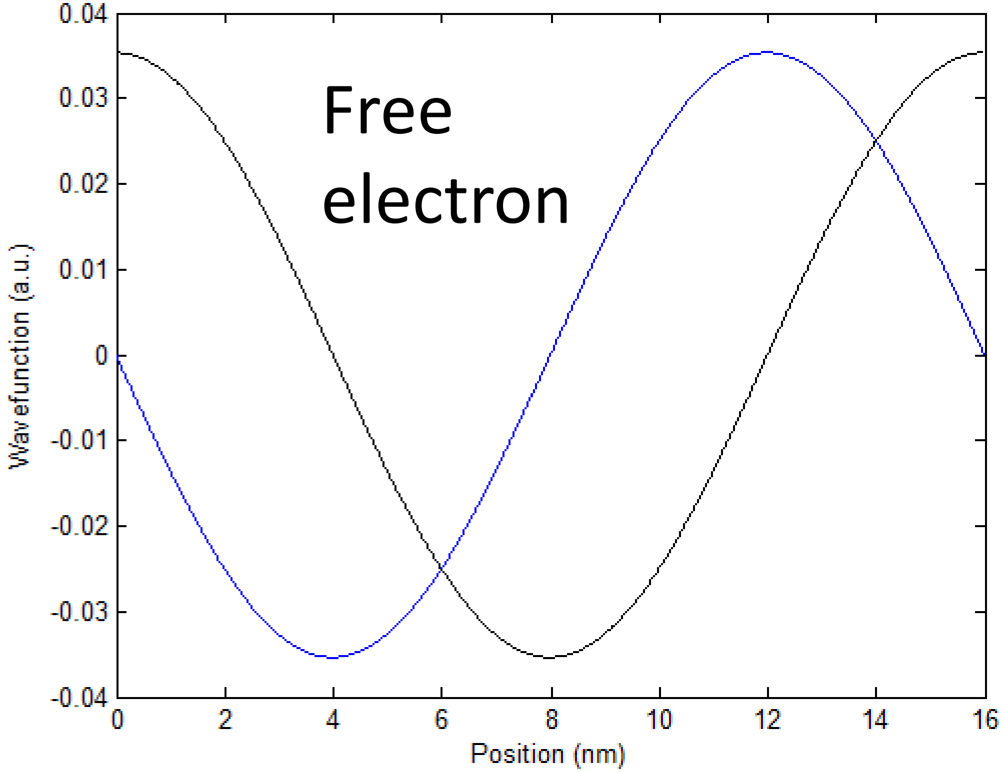




Wavefunction (Periodic potential well)

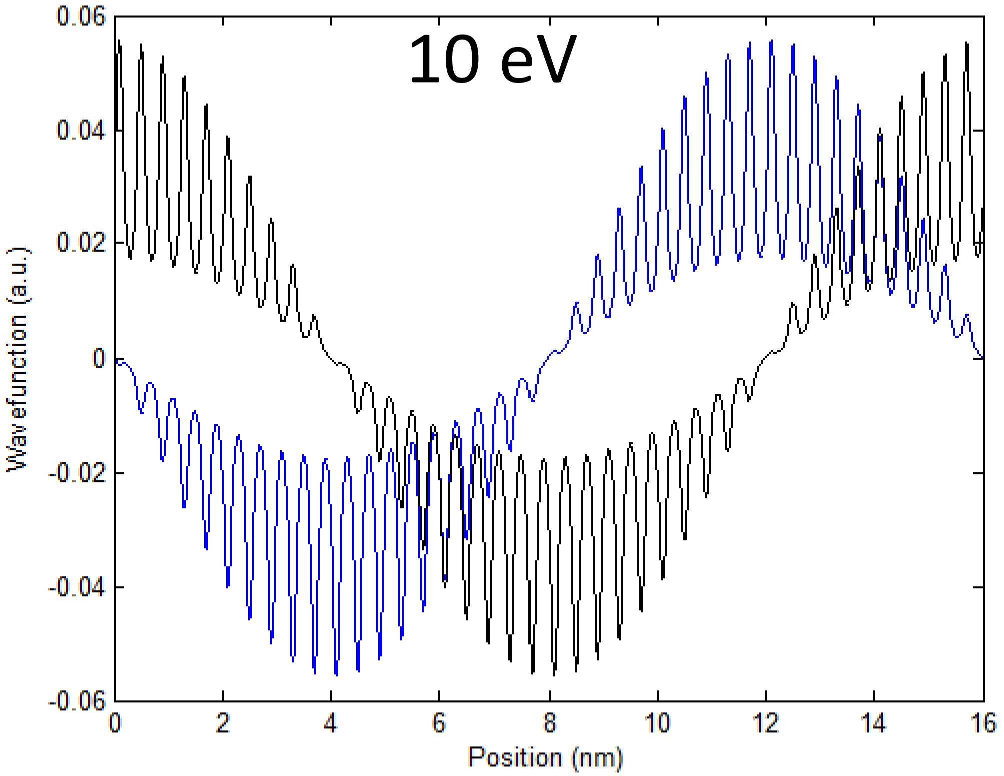
- When a is 0.4 nm, N is 40, the well width is 10 nm, and the well depth is 10.0 eV,

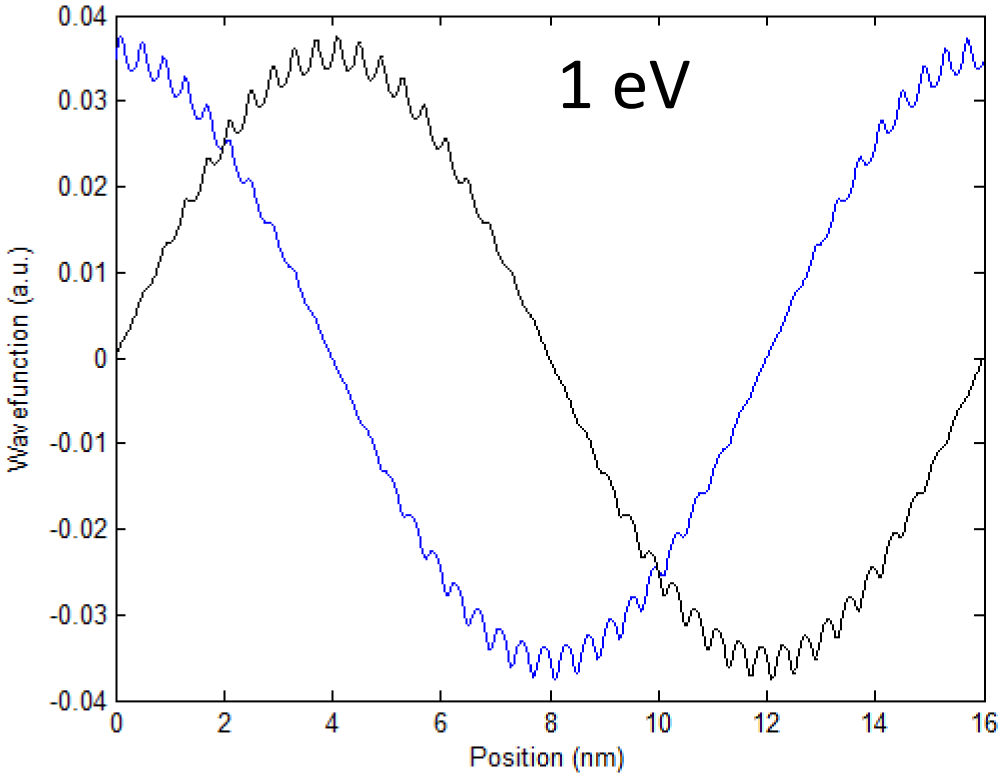




Observation

- $\psi(x)$ in a periodic potential well is a modulated version of the free electron wave function.





Bloch theorem

- Under a periodic potential, the wavefucntion can be expressed in a form of

$$\psi(\mathbf{r}) = u(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$$

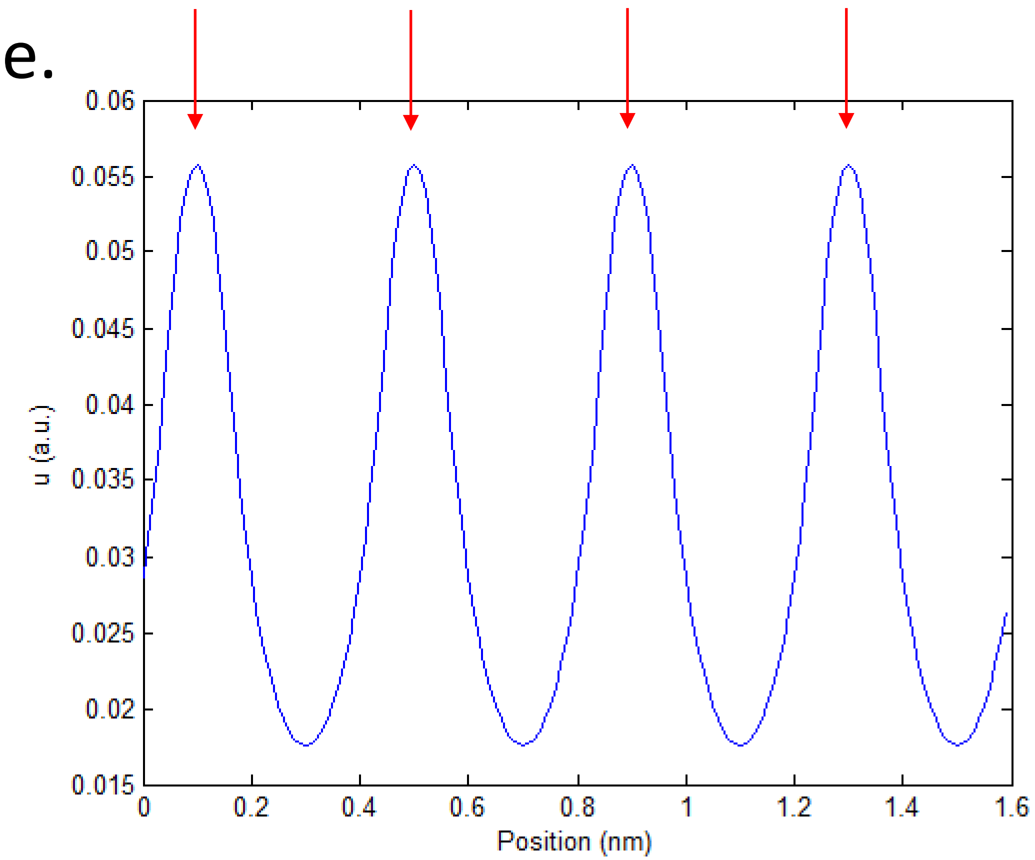
  – $u(\mathbf{r})$ is periodic within the direct lattice.

  $u(\mathbf{r}+\mathbf{R}) = u(\mathbf{r})$

  $\mathbf{R} = i\mathbf{a}_1 + j\mathbf{a}_2 + k\mathbf{a}_3$

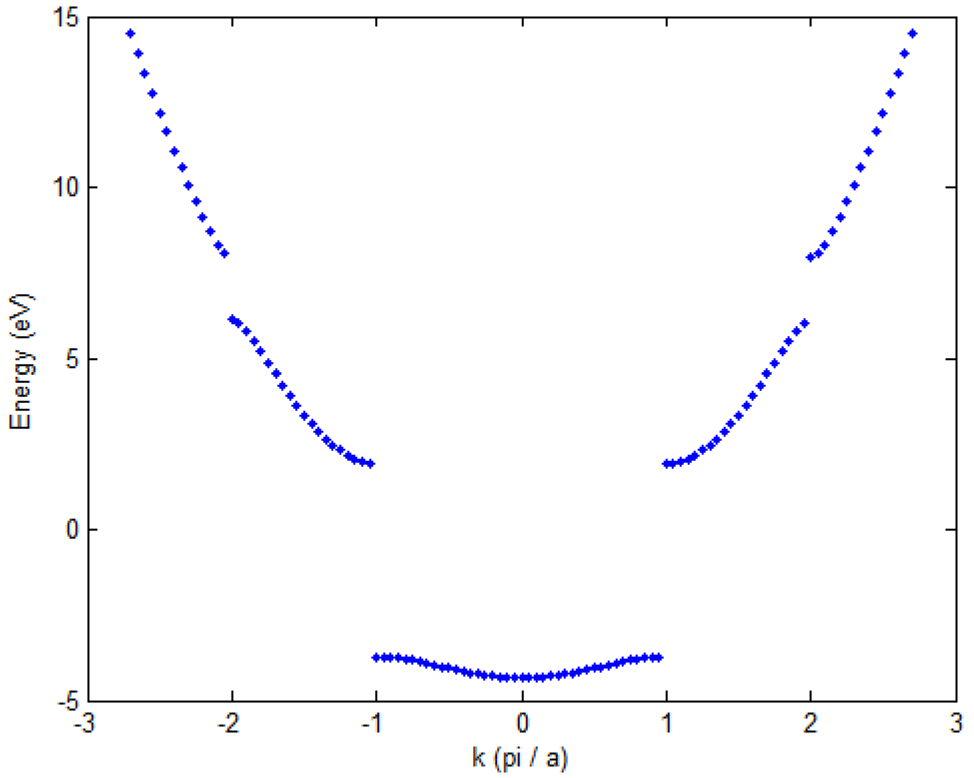
  – $\mathbf{k}$ can be used to identify a state, still.

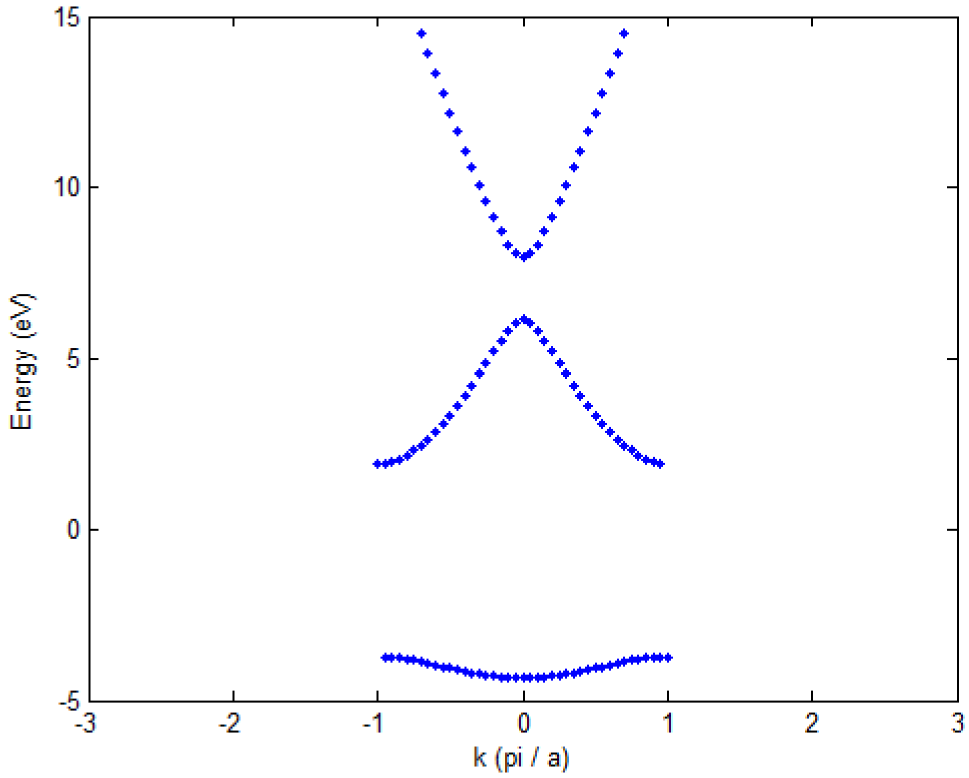
10 eV, $k = \frac{2\pi}{Na} \times 1$



Reduced zone scheme

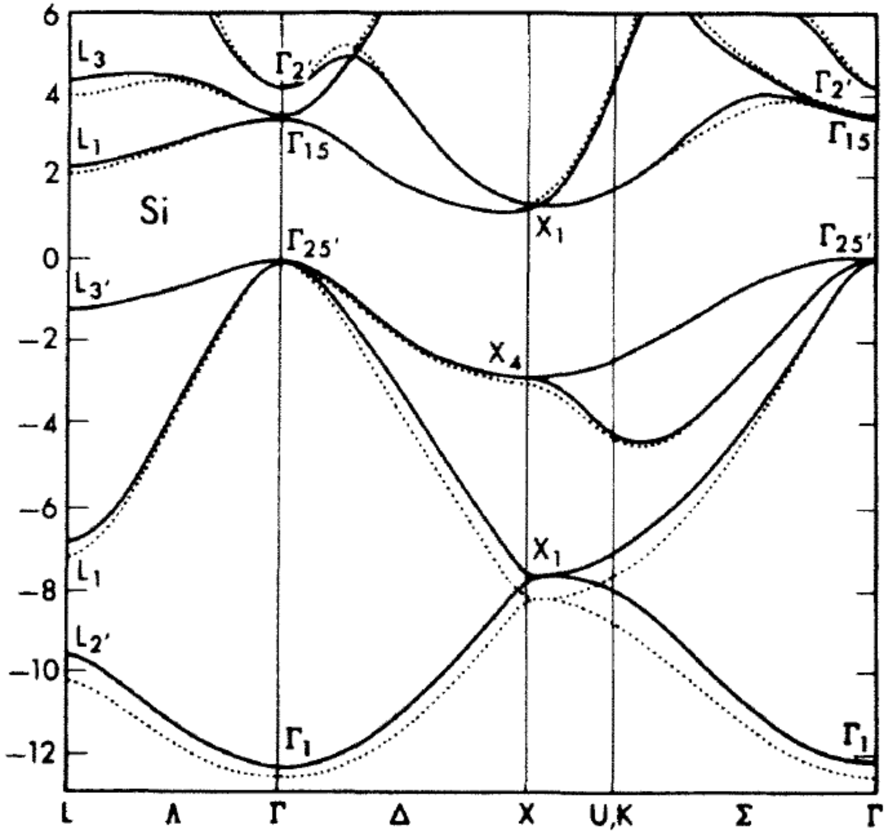
- When $\mathbf{k}$ is outside the first BZ, it is mapped onto the first BZ.

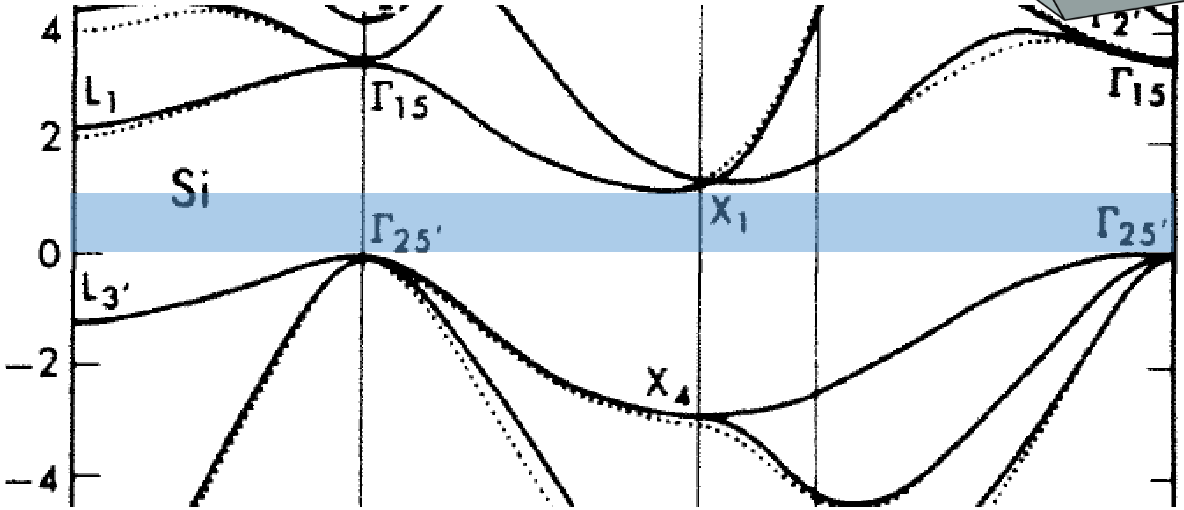


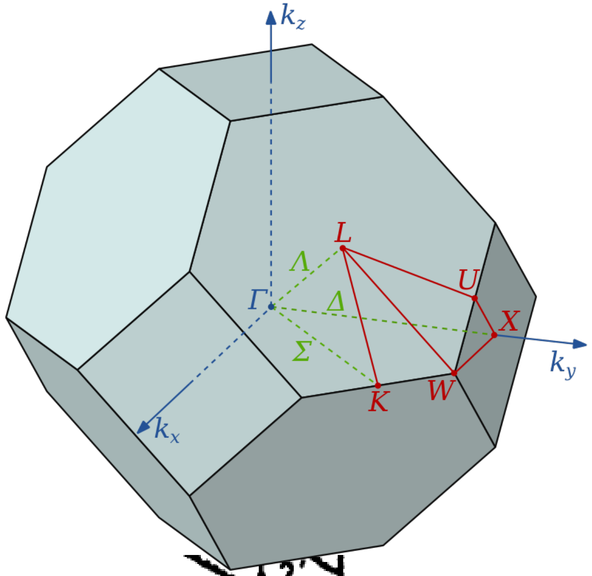


Band structure

- We can draw the $E - k$ diagram.
  - Bandgap is found.

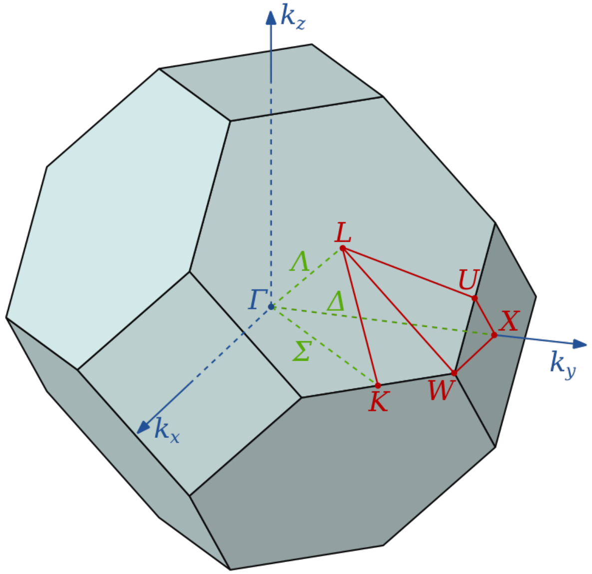






Silicon band structure
(Chelikowsky and Cohen, PRB, vol. 14, p. 556, 1976)

Velocity and inverse mass



- Velocity

$$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar} \nabla_k E(\mathbf{k})$$

- Inverse mass (its ij component)

$$m_{ij}^{-1} = \frac{1}{\hbar} \frac{\partial}{\partial k_i} \frac{\partial}{\partial k_j} E(\mathbf{k})$$

- Example) Silicon conduction band

$$E(\mathbf{k}) - E_c = \frac{\hbar^2}{2} \left(\frac{1}{m_{xx}} k_x^2 + \frac{1}{m_{yy}} k_y^2 + \frac{1}{m_{zz}} k_x^2 \right)$$ ~ Taur, Eq. (2.2)

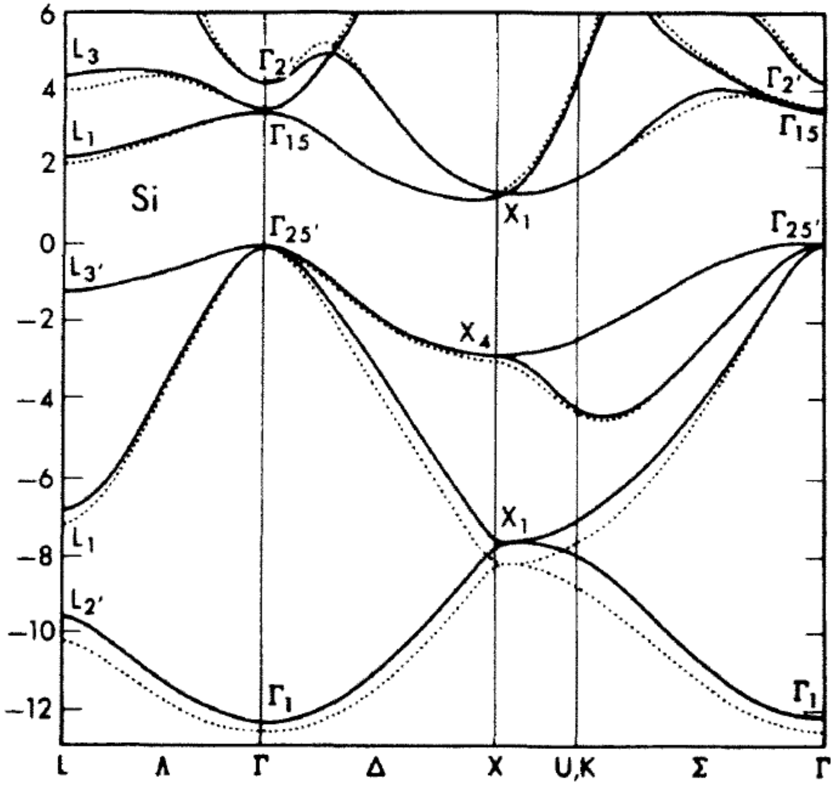
  – Among three masses, one is m_l and the other two are m_t.

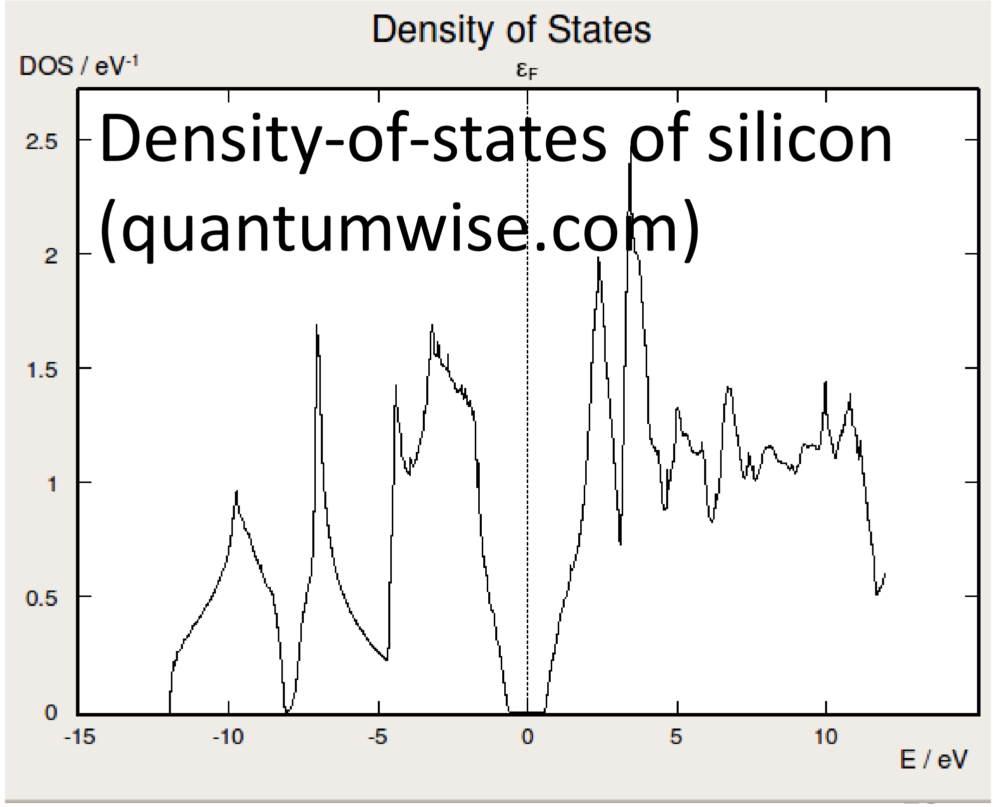
Density-of-states (DOS)

- DOS, $N(E)$, (per spin, per valley)

$$N(E)dE = \frac{1}{(2\pi)^3} dk_x dk_y dk_z$$

~ Taur, Eq. (2.1)





Density-of-states of silicon (quantumwise.com)

Density-of-states (DOS) of an ellipsoidal valley

- Volume in the $\mathbf{k}$-space
  - For simplicity, assume that E_c is 0. With $m^* = \left(m_{xx}m_{yy}m_{zz}\right)^{\frac{1}{3}}$,

$$\frac{4\pi}{3}\left(\frac{1}{\hbar}\right)^3 (2m^*)^{1.5}(E)^{1.5}$$

  - Therefore, within a range between E and $E + dE$, the volume is

$$4\pi\left(\frac{1}{\hbar}\right)^3 \left(2m_{xx}m_{yy}m_{zz}\right)^{0.5}(E)^{0.5}dE$$

- DOS of silicon conduction band (per spin, per valley)

$$N(E)dE = \frac{4\pi}{h^3}(2m_l m_t^2)^{0.5}(E)^{0.5}dE$$

~ Taur, Eq. (2.3)

Thank you!